

Peculiarities of the electro- and magnetoresistivity of WTe_2 and MoTe_2 single crystals before and after quenching

Cite as: AIP Advances **11**, 015226 (2021); <https://doi.org/10.1063/9.0000182>

Submitted: 15 October 2020 . Accepted: 25 November 2020 . Published Online: 11 January 2021

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Presented: 4 November 2020 • Submitted: 15 October 2020 •
Accepted: 25 November 2020 • Published Online: 11 January 2021



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Note: This paper was presented at the 65th Annual Conference on Magnetism and Magnetic Materials.

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ABSTRACT

WTe_2 and MoTe_2 single crystals were grown, some of them were quenched, and the following properties were studied: electroresistivity in the temperature range from 1.8 to 300 K, magnetoresistivity at temperatures from 1.8 to 300 K in magnetic fields of up to 9 T. On the one hand, quenching leads to dramatic changes in the behaviour and value of the electroresistivity of MoTe_2 ; the type of the electroresistivity changes from “semiconductor” to “metallic”, and the electroresistivity values of MoTe_2 before and after quenching differ by 8 orders of magnitude (!) at low temperatures. On the other hand, quenching is shown not to lead to significant changes in the behaviour and value of the electroresistivity of WTe_2 . A relatively small increase in the electroresistivity of quenched WTe_2 at low temperatures can be associated with the scattering of current carriers by structural defects. The magnetoresistivity of MoTe_2 increases from 7 to 16% in a field of 9 T at a temperature of 12 K as a result of quenching. The magnetoresistivity of WTe_2 is shown to reach ~1700% in a field of 9 T at 2 K. The behaviour of the magnetoresistivity of non-quenched samples is typical for compensated conductors with a closed Fermi surface.

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I. INTRODUCTION

Topological Weyl semimetals (TWSs) based on transition metal dichalcogenides (TMDs) are of great interest both from fundamental and applied points of view (Refs. 1–6). Such materials have promising prospects for use in spintronics and micro- and nano-electronics due to unusual electronic and magnetic properties owing to their unique band structure, such as extremely large magnetoresistance, high charge carrier mobility, and spin-polarized transport. In particular, quasiparticles in the bulk of TWSs are massless Weyl fermions. They can be controlled much faster than ordinary charge carriers due to “zero” effective mass. The unique spin-polarized surface states in TWSs are called Fermi arcs. TMD WTe_2 and MoTe_2 were found to exhibit the TWS features (Refs. 3 and 4). Moreover, the physical properties of MoTe_2 are known to strongly depend on

the type of crystal structure that can be tuned by heat treatment (Refs. 7–9). MoTe_2 undergoes a transition from the diamagnetic semiconductor phase to the paramagnetic semimetallic one under certain conditions. Hence, it is of interest to track these changes in MoTe_2 and investigate how quenching affects the crystal and electronic structure of the WTe_2 compound, in particular, the electro- and magnetoresistivity. Therefore, the purpose of this work is to study the electro- and magnetoresistivity of WTe_2 and MoTe_2 single crystals before and after quenching.

II. EXPERIMENTAL

WTe_2 single crystals were grown by the chemical vapour transport method using Br_2 as a transport agent according to the procedure described in Ref. 8. In order to study the effect of quenching on

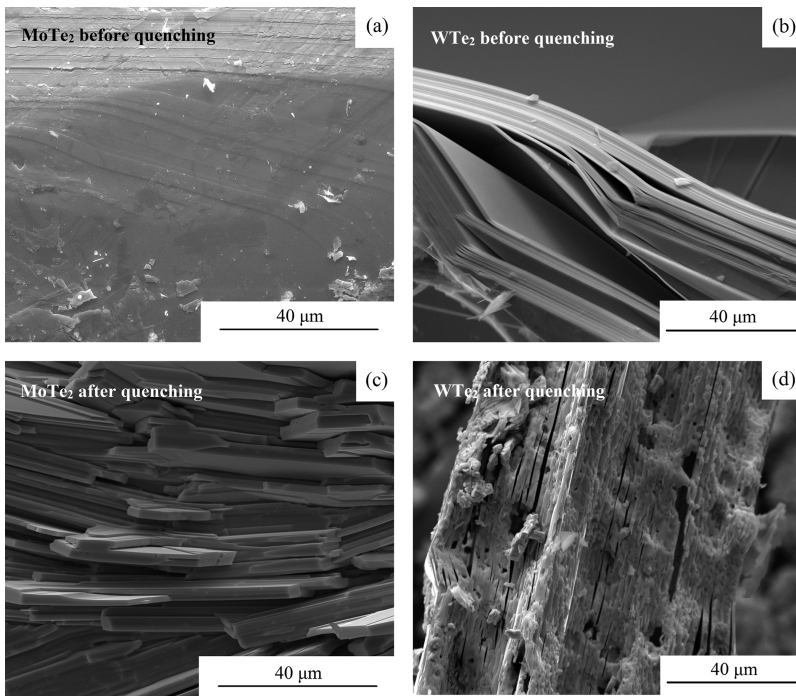


Figure 1. The SEM images of MoTe₂ (a, c) and WTe₂ (b, d) before and after quenching, respectively.

the crystal structure and electronic transport of obtained samples, some single crystals were sealed in a quartz ampoule, then heated to 910°C, held at this temperature for 1 hour, and quenched in water.

X-ray diffraction analysis revealed that MoTe₂ crystallizes in a hexagonal structure with the lattice parameters $a = 3.540(7)$ Å and $c = 13.983(5)$ Å. The parameter c changes noticeably after quenching to ~ 13.81 Å. Such values of the parameter c before and after quenching are close to its values for α -MoTe₂ (hexagonal) and β -MoTe₂ (monoclinic), respectively (Refs. 10–12), that may indicate the structural transition that occurred during quenching. While WTe₂ crystallizes in a orthorhombic structure with the lattice parameters $a = 3.435(8)$ Å, $b = 6.312(7)$ Å and $c = 14.070(4)$ Å. No significant changes in the crystal structure of WTe₂ after quenching are observed.

The chemical composition of the samples and microstructure of their surface were investigated using a FEI Inspect F scanning electron microscope (SEM) equipped with an EDAX attachment for

X-ray microanalysis. Figure 1 shows the SEM images of MoTe₂ and WTe₂ before and after quenching. In the case of MoTe₂ (figure 1a, c), we can observe an increase in the layering of the sample after quenching. The layer thickness is approximately 1.5 μm. In the case of WTe₂ (figure 1b, d), an increase in the number of defects of the sample after quenching can be noted.

The temperature dependences of the electro- and magnetoresistivity were measured by the standard method (see, e.g. Refs. 13 and 14) in the temperature range from 1.8 to 300 K in magnetic fields of up to 9 T. The measurements were carried out using the PPMS-9 system (Quantum Design) in Collaborative Access Center “Testing Center of Nanotechnology and Advanced Materials” of IMP, UB of RAS.

III. RESULT AND DISCUSSIONS

Figure 2 shows the temperature dependences of the electroresistivity $\rho_0(T)$ of MoTe₂ (figure 2a) and WTe₂ (figure 2b) before and after quenching.

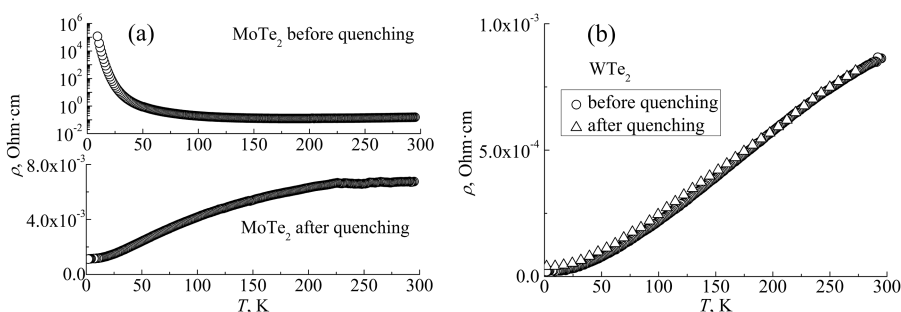


Figure 2. The temperature dependences of the electroresistivity of MoTe₂ (a) and WTe₂ (b) before and after quenching.

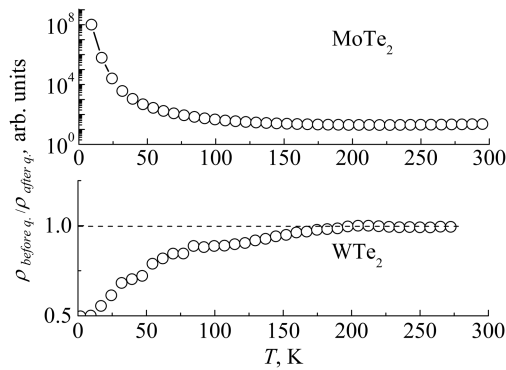


Figure 3. The temperature dependences of the relationship of the electroresistivity of MoTe₂ and WTe₂ before quenching to the electroresistivity after one.

and after quenching in the temperature range from 1.8 to 300 K. The dependence $\rho_0(T)$ of non-quenched MoTe₂ (figure 2a) is seen to have a “semiconductor” type with a very large resistivity value of more than 10^5 Ohm cm at low temperatures, whereas the resistivity is less than 1 Ohm cm at temperatures above 50 K. The dependence $\rho_0(T)$ of quenched MoTe₂ shows a “metallic” behaviour with a resistivity value of $\sim (1.1\text{--}6.8) \cdot 10^{-3}$ Ohm cm, that is 8 orders of magnitude (!) less than the resistivity of MoTe₂ before quenching at low temperatures. Thus, quenching leads to the dramatic change in the electroresistivity of MoTe₂. The analysis of the behaviour of electroresistivity of MoTe₂ before and after quenching is presented in Ref. 15. The dependence $\rho_0(T)$ of WTe₂ (figure 2b) has a “metallic” type with a resistivity value of $\sim (0.2\text{--}8.6) \cdot 10^{-4}$ Ohm cm, monotonically increasing with temperature according to a law close to quadratic at low temperatures, reaching a linear dependence at $T > 60$ K with a tendency to saturation at temperatures above 240 K. Quenching is seen to do not lead to significant changes in the behaviour and value of the electroresistivity of WTe₂.

Figure 3 shows the temperature dependences of the relationship of the electroresistivity before quenching to the electroresistivity after one $\rho_{\text{before } q} / \rho_{\text{after } q}$. In the case of MoTe₂, the dependence $\rho_{\text{before } q} / \rho_{\text{after } q}$ reaches 10^8 arb. units at low temperatures and decreases with temperature. While, in the case of WTe₂, the value of $\rho_{\text{before } q} / \rho_{\text{after } q}$ is less than 1 at low temperatures, and tends to 1 at high temperatures, which can be due to the scattering of current carriers by structural defects in WTe₂ after quench-

ing at low temperatures. At the same time, at high temperatures, phonons have the main contribution in scattering. Therefore, these graphs demonstrate the dramatic differences in the behaviour of the electroresistivity of MoTe₂ and WTe₂ before and after quenching.

Figure 4 shows the field dependences of the magnetoresistivity (MR) $\Delta\rho_{xx}/\rho_0(B)$ of MoTe₂ before and after quenching and WTe₂ in magnetic fields of up to 9 T at temperatures of 12 K and 2 K, respectively. The MR was calculated by the formula

$$\Delta\rho_{xx}/\rho_0 = (\rho_{xx} - \rho_0)/\rho_0 \times 100\%, \quad (1)$$

where ρ_0 is the electroresistivity without a magnetic field, ρ_{xx} is the resistivity in magnetic fields of up to 9 T. The dependence $\Delta\rho_{xx}/\rho_0(B)$ of MoTe₂ before quenching is close to quadratic and about 7% in a field of 9 T (figure 4a). The quadratic dependence $\Delta\rho_{xx}/\rho_0(B)$ is known to be characteristic of compensated conductors with a closed Fermi surface Ref. 16. Quenching is seen to lead to an increase in the MR to $\sim 16\%$, and along with the quadratic field contribution, the linear term also appears. The linear on a magnetic field contribution to the MR can be due to the appearance of open electron orbits perpendicular to the direction of the electric current in reciprocal space Ref. 16. Figure 4b shows the field dependence of the MR of WTe₂. The MR increases with a field and reaches $\sim 1700\%$ at 2 K in a field of 9 T. The analysis of the dependence $\Delta\rho_{xx}/\rho_0(B)$ of WTe₂ revealed that, since the MR changes according to a law close to quadratic in fields of up to 9 T, such a behavior of the MR is typical for compensated conductors with a closed Fermi surface in the region of strong effective magnetic fields Ref. 16.

It should be noted that the magnitude of the MR of WTe₂ is 2 orders of magnitude higher than that the MR of MoTe₂ (Figure 4). This is largely due to the difference in the “electrical” purity of the crystals, i.e. Residual Resistance Ratio (RRR), where $RRR = \rho_{295\text{ K}}/\rho_{2\text{ K}}$. For WTe₂, $RRR \approx 43$, and for MoTe₂ after quenching, $RRR \approx 6$. Thus, in the case of the WTe₂ single crystal, the range of magnetic fields of up to 9 T, where the close-to-quadratic magnetic field dependence of the MR is observed, refers to the region of high effective magnetic fields with $\omega\tau \gg 1$ (ω is the cyclotron frequency, τ is the relaxation time) with a strong dependence on B and a large MR Ref. 16. A similar strong dependence $\Delta\rho_{xx}/\rho_0(B)$ with a large MR was observed in the Ref. 17. For the MoTe₂ single crystal after quenching, magnetic fields of up to 9 T are apparently intermediate, where $\omega\tau \sim 1$, with the weaker dependence $\Delta\rho_{xx}/\rho_0(B)$ and the significantly lower MR.

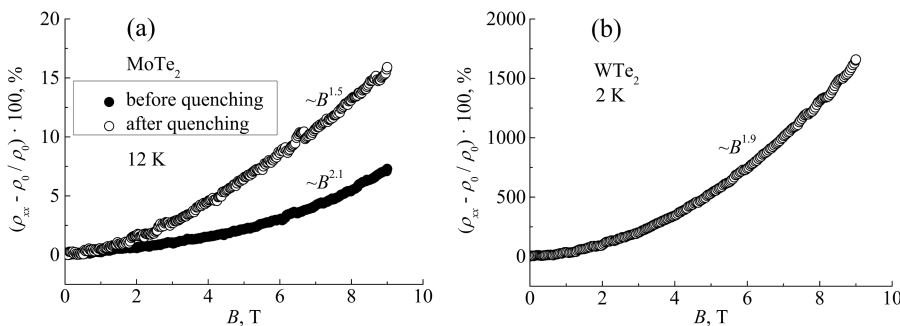


Figure 4. The field dependences of the MR of MoTe₂ before and after quenching (a) and WTe₂ (b) in magnetic fields of up to 9 T at temperatures of 12 K and 2 K, respectively.

IV. CONCLUSIONS

The studies of the electro- and magnetoresistivity of WTe_2 and MoTe_2 single crystals before and after quenching allow us to draw the following conclusions. On the one hand, quenching leads to the dramatic changes in the behaviour and value of the electroresistivity of MoTe_2 : the type of the electroresistivity changes from “semiconductor” to “metallic”, and the electroresistivity value of MoTe_2 decreases by 8 orders of magnitude (!) from $\sim 10^5$ to $\sim 10^{-3}$ Ohmcm at low temperatures. On the other hand, quenching is shown to do not lead to significant changes in the behaviour and value of the electroresistivity of WTe_2 : the type of the temperature dependence of the electroresistivity is “metallic”, and its value increases from $0.2 \cdot 10^{-4}$ to $8.6 \cdot 10^{-4}$ Ohm cm in the temperature range from 1.8 to 300 K. A relatively small increase in the electroresistivity of quenched WTe_2 at low temperatures can be associated with the scattering of current carriers by structural defects, which are also reflected by the data of scanning electron microscopy. The MR of MoTe_2 increases from 7 to 16% in a field of 9 T at a temperature of 12 K as a result of quenching. The MR of WTe_2 is shown to reach $\sim 1700\%$ in a field of 9 T at 2 K. The behaviour of the MR of non-quenched samples is typical for compensated conductors with a closed Fermi surface.

ACKNOWLEDGMENTS

The research was carried out within the state assignment of Ministry of Education and Science of the Russian Federation (theme “Spin”, No. AAAA-A18-118020290104-2), supported in part by RFBR (Project No. 20-32-90069) and the Government of the Russian Federation (Decree No. 211, Contract No. 02.A03.21.0006).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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